

Ta ₂₁ Te ₁₃	<i>hP</i> 136	(183) <i>P6mm</i> – f ² e ¹¹ d ⁶ cb ² a ³
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Ta₂₁Te₁₃ [1]

Structural features: Heavily corrugated slabs consisting of three Ta layers between two Te layers. Ta₁₅₁ clusters formed by nineteen fused TaTa₁₂ hexagonal antiprisms.

Conrad M. et al. (2000) [1]

Ta₂₁Te₁₃

$a = 1.95$, $c = 1.03$ nm, $c/a = 0.528$, $V = 3.3919$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	12 <i>f</i>	1	0.084	0.415	0.521		icosahedron Ta ₈ Te ₄
Ta2	12 <i>f</i>	1	0.144	0.428	0.259		icosahedron Te ₃ Ta ₉
Ta3	6 <i>e</i>	. <i>m</i> .	0.083	0.917	0.368		icosahedron Ta ₉ Te ₃
Te4	6 <i>e</i>	. <i>m</i> .	0.113	0.887	0.929		non-coplanar triangle Ta ₃
Ta5	6 <i>e</i>	. <i>m</i> .	0.145	0.855	0.179		icosahedron Te ₄ Ta ₈
Ta6	6 <i>e</i>	. <i>m</i> .	0.162	0.838	0.45		icosahedron Te ₃ Ta ₉
Te7	6 <i>e</i>	. <i>m</i> .	0.198	0.802	0.692		icosahedron Ta ₄ Te ₈
Te8	6 <i>e</i>	. <i>m</i> .	0.222	0.778	0.031		pseudo Frank-Kasper Ta ₄ Te ₇
Ta9	6 <i>e</i>	. <i>m</i> .	0.25	0.75	0.478		icosahedron Te ₃ Ta ₉
Ta10	6 <i>e</i>	. <i>m</i> .	0.286	0.714	0.219		icosahedron Te ₄ Ta ₈
Te11	6 <i>e</i>	. <i>m</i> .	0.395	0.605	0.64		14-vertex Frank-Kasper Ta ₇ Te ₇
Ta12	6 <i>e</i>	. <i>m</i> .	0.422	0.578	0.386		14-vertex Frank-Kasper Te ₂ Ta ₁₂
Te13	6 <i>e</i>	. <i>m</i> .	0.433	0.567	0.123		single atom Ta
Ta14	6 <i>d</i>	.. <i>m</i>	0.145	0	0.136		icosahedron Ta ₈ Te ₄
Te15	6 <i>d</i>	.. <i>m</i>	0.202	0	0.573		single atom Ta
Ta16	6 <i>d</i>	.. <i>m</i>	0.265	0	0.341		14-vertex Frank-Kasper Te ₂ Ta ₁₂
Te17	6 <i>d</i>	.. <i>m</i>	0.32	0	0.096		14-vertex Frank-Kasper Ta ₇ Te ₇
Te18	6 <i>d</i>	.. <i>m</i>	0.404	0	0.754		non-coplanar triangle Ta ₃
Ta19	6 <i>d</i>	.. <i>m</i>	0.429	0	0.298		icosahedron Ta ₉ Te ₃
Ta20	3 <i>c</i>	2 <i>mm</i>	¹ / ₂	0	0.546		icosahedron Te ₄ Ta ₈
Te21	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.0		non-coplanar triangle Ta ₃
Ta22	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.456		icosahedron Te ₃ Ta ₉
Te23	1 <i>a</i>	6 <i>mm</i>	0	0	0.0		single atom Ta
Ta24	1 <i>a</i>	6 <i>mm</i>	0	0	0.263		14-vertex Frank-Kasper Te ₂ Ta ₁₂
Te25	1 <i>a</i>	6 <i>mm</i>	0	0	0.52		single atom Ta

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.06

Experimental: polycrystalline sample, electron diffraction

Remarks: Hexagonal approximant of dodecagonal dd-Ta_{1.6}Te quasicrystals. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Conrad M., Krumeich F., Reich C., Harbrecht B. (2000), Mater. Sci. & Eng. A 294/296, 37-40.